Methyl acetate

| Welliyi acelale | | | | | | | | |
|-----------------|---------------|--|--|--|--|--|--|--|
| 79-20-9 | DTXSID4021767 | | | | | | | |
| | | | | | | | | |

Model Performance

| Model | Data | | |
|-------|------|--|--|

Weighted KNN model

| 5-fold CV (| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-------------|-----------------|------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 | |

Model Results

Predicted value: 7.22 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.46e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

Image not found

Acrylamide Measured: 50.1 Predicted: 16.7 Image not found

Acetic acid
Measured: 1.00
Predicted: 2.40

Image not found

1,2-Propylene glycol Measured: 2.29 Predicted: 4.24

Image not found

1,4-Dioxane Measured: 17.0 Predicted: 13.2 Image not found

Acetamide
Measured: 5.01
Predicted: 4.44